allenCahn formulation

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1 Outline

The weak formulations corresponding to the generic coupled phase field problem are derived, including the effects of interface energy anisotropy, but assuming isotropic mobility. Also, for now, the change in the normal direction due to mechanical deformation has not been included. The formulation will soon be extended to include variations of $\boldsymbol{n}$ and anisotropic tensorial mobility.

2 Variational formulation

The total free energy of the system (neglecting boundary terms) is of the form,

$$\Pi(\eta) = \int_{\Omega_0} F(\eta)\ JdV \tag{1}$$

where dV represents a volume element in the reference configuration, $J = \det\boldsymbol{F}$ is the local volume change ratio and the free energy density is given by

$$F(\eta) = \left(f(\eta) + \frac{1}{2}\nabla\eta \cdot\ \boldsymbol{\kappa}^{\eta}\ \nabla\eta \right) \tag{2}$$

Now we proceed to derive the governing equations in the weak form.

3 Allen-Cahn governing equations

Considering variations of the form $\eta_\epsilon = \eta + \epsilon\omega$, the first variation of the free energy with respect to the order parameter, η, is given by:

$$\begin{aligned} \delta_\eta\Pi &= \left.\frac{d\Pi(\eta+\epsilon\omega)}{d\epsilon}\right|_{\epsilon=0} \\ &= \int_{\Omega_0} \frac{\partial f}{\partial\eta}\ \omega\ JdV \\ &+ \int_{\Omega_0} \kappa^{\eta}\ \eta_{,i}\ \omega_{,i}\ JdV \end{aligned} \tag{3}$$

Integration by parts gives:

$$\begin{aligned} \delta_c\Pi = &\int_{\Omega_0} \frac{\partial f}{\partial\eta}\ \omega\ JdV \\ - &\int_{\Omega_0} (\ \kappa^{\eta}\ \eta_{,i}\ )_{,i}\ \omega\ JdV + \int_{\Gamma_0} \kappa^{\eta}\ \eta_{,i}\ n_i\ \omega\ JdS \end{aligned} \tag{4}$$

Collecting terms:

$$
\begin{aligned}
\delta_c \Pi = & \int_{\Omega_0} \omega \left[\frac{\partial f}{\partial c} \right] JdV \\
& + \int_{\Gamma_0} \omega \ \kappa^c \ c_{,i} \ n_i \ JdS
\end{aligned} \tag{5}
$$

From non-equilibrium thermodynamics we know that the volume integrand represents the chemical potential,

$$
\zeta = \frac{\partial f}{\partial \eta} - \zeta^{grad} \tag{6}
$$
$$
\text{where} \quad \zeta^{grad} = (\chi_i^\eta)_{,i} \quad \text{and} \quad \chi_i^\eta = \kappa^\eta \ \eta_{,i}
$$

3.1 Governing equation

The governing equation for the non-conserved structural order parameter is given by:

$$
\frac{\partial \eta}{\partial t} + L^\eta \zeta = 0 \tag{7}
$$

Again the mobility is assumed to be a constant scalar. Now the corresponding weak form is given by:

$$
\begin{aligned}
& \int_{\Omega_0} \omega \ \left[\frac{\partial \eta}{\partial t} + L^\eta \zeta \right] \ JdV = 0 \\
\Rightarrow & \int_{\Omega_0} \omega \ \left[\frac{\partial \eta}{\partial t} + L^\eta \ \left(\frac{\partial f}{\partial \eta} - (\chi_i^\eta)_{,i} \right) \right] \ JdV = 0
\end{aligned} \tag{8}
$$

Integration by parts gives the following formulation for order parameter dynamics:

$$
\Rightarrow \int_{\Omega_0} \omega \frac{\partial \eta}{\partial t} \ JdV + \int_{\Omega_0} \omega \ L^\eta \frac{\partial f}{\partial \eta} \ JdV + \int_{\Omega_0} \omega_{,i} \ L^\eta \ \chi_i^\eta \ JdV - \int_{\Gamma_0} \omega \ L^\eta \ \chi_i^\eta \ n_i \ JdS = 0 \tag{9}
$$

However this is not the full weak form, because if we try to obtain the strong form starting with Equation (9) we simply revert to Equation (8) which only has the PDE without information about the boundary conditions. So with the knowledge of the boundary condition terms from Equation (9), we obtain the consistent weak formulation by adding an additional surface integral term to Equation (9),

$$
\begin{aligned}
\Rightarrow & \int_{\Omega_0} \omega \frac{\partial \eta}{\partial t} \ JdV + \int_{\Omega_0} \omega \ L^\eta \frac{\partial f}{\partial \eta} \ JdV + \int_{\Omega_0} \omega_{,i} \ L^\eta \ \chi_i^\eta \ JdV - \int_{\Gamma_0} \omega \ L^\eta \ \chi_i^\eta \ n_i \ JdS \\
& + \int_{\Gamma_0} \omega \ L^\eta \ \left(\chi_i^\eta \ n_i - \mathcal{J}^\eta \right) \ JdS = 0
\end{aligned} \tag{10}
$$

where $\mathcal{J}^\eta$ is the boundary flux term. The resulting consistent weak formulation is given by:

$$
\Rightarrow \int_{\Omega_0} \omega \frac{\partial \eta}{\partial t} \ JdV + \int_{\Omega_0} \omega \ L^\eta \frac{\partial f}{\partial \eta} \ JdV + \int_{\Omega_0} \omega_{,i} \ L^\eta \ \chi_i^\eta \ JdV - \int_{\Gamma_0} \omega \ L^\eta \mathcal{J}^\eta \ JdS = 0 \tag{11}
$$